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Ionization amplitude for e-H collision near threshold with three Coulomb final state wave function

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Abstract : In this work, we evaluate the matrix element for electron impact ionization of atomic hydrogen near the threshold, wherein the final state wave function is a product of three-Coulomb functions which is asymptotically exact Since the normalisation factor of the part of the wave function corresponding to electron-electron repulsive interaction vanishes exponentially at threshold, it was thought uptill now that the matrix element also would vanish exponentially We however, have shown that this exponential factor is compensated for

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There is a long standing idea [1] that the matrix element for electron impact ionization will vanish exponentially at threshold when the final state is represented by a product of three Coulomb functions [2] which is known to be asymptotically correct. This unphysical behaviour has been attributed to the exponential vanishing of the normalisation factor of that part of the wave function describing the repulsive electron-electron interaction. In this work we have worked out the detailed evaluation of the matrix element to show how this exponential factor is appropriately compensated for and a physical result is obtained.

The matrix element for electron impact ionization of hydrogen atom is given (in atomic unit) by [3]

$$M = (1/2\pi)\left\langle \psi_f^- \middle| V_i \middle| \psi_i \right\rangle \tag{1}$$

where

$$V_i = -\frac{1}{r_1} + \frac{1}{r_{12}}, \tag{2}$$

$$r_{12} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|;$$

$\boldsymbol{r}_1, \boldsymbol{r}_2$ are the position vectors of the projectile and target electrons respectively.

ψ_i is the initial state wave function, given by

$$\psi_i = (1/\sqrt{\pi}) \exp(-\lambda r_2) \exp(i\boldsymbol{k}_i . \boldsymbol{r}_1) \tag{3}$$

and ψ_f^-, the properly normalised final state wave function near the threshold, involves a product of three confluent hypergeometric functions :

$$\begin{aligned}\psi_f^-(\boldsymbol{r}_1, \boldsymbol{r}_2) = {} & \left(\alpha_1\alpha_2\alpha_3\right)^{1/2} \exp\left(-\pi\alpha_3\right) \exp\left(i\boldsymbol{k}_1.\boldsymbol{r}_1 + i\boldsymbol{k}_2.\boldsymbol{r}_2\right) \\ & \times {}_1F_1\left[-i\alpha_1, 1, -i(k_1 r_1 + \boldsymbol{k}_1.\boldsymbol{r}_1)\right] \times {}_1F_1\left[-i\alpha_2, 1, -i(k_2 r_2 + \boldsymbol{k}_2.\boldsymbol{r}_2)\right] \\ & \times {}_1F_1\left[i\alpha_3, 1, -i(q r_{12} + \boldsymbol{q}.\boldsymbol{r}_{12})\right],\end{aligned} \tag{4}$$

$\boldsymbol{k}_i$, $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ are respectively the momenta of the incident, scattered and ejected electrons.

Here, $\alpha_1 = 1/k_1, \ \alpha_2 = 1/k_2, \ \alpha_3 = 1/|\boldsymbol{k}_1 - \boldsymbol{k}_2| = 1/2q.$

In view of eqs. (2), (3) and (4) and the contour integral representation of the confluent hypergeometric function [4]

$${}_1F_1(i\alpha, 1, z) = (1/2\pi i) \oint \exp(zt)\, t^{-1+i\alpha} (t-1)^{-i\alpha}\, dt,$$

eq. (1) can be written as

$$M = \left[(1/4\pi^3)\alpha_1\alpha_2\alpha_3\right]^{1/2} \exp(-\pi\alpha_3) \times I. \tag{5}$$

where
$$\begin{aligned} I = {} & \int \exp\left[i(\boldsymbol{k}_i - \boldsymbol{k}_1).\, \boldsymbol{r}_1 - i\boldsymbol{k}_2.\boldsymbol{r}_2 - \lambda r_2\right]\left(1/r_1 - 1/r_{12}\right) \times \left[1/(2\pi i)^3\right] \\ & \times \oint\oint\oint dt_1 dt_2 dt_3\, t_1^{i\alpha_1 - 1}(t_1 - 1)^{-i\alpha_1} \times t_2^{i\alpha_2 - 1}(t_2 - 1)^{-i\alpha_2} \times t_3^{i\alpha_3 - 1}(t_3 - 1)^{i\alpha_3} \\ & \times \exp\left[i\{(k_1 r_1 + \boldsymbol{k}_1.\boldsymbol{r}_1)t_1 + (k_2 r_2 + \boldsymbol{k}_2.\boldsymbol{r}_2)t_2 + (q r_{12} + \boldsymbol{q}.\boldsymbol{r}_{12})t_3\}\right] d\boldsymbol{r}_1 d\boldsymbol{r}_2.\end{aligned} \tag{6}$$

The integral I can be derived from a mother integral I_1, *i.e.*

$$I = \underset{\substack{\eta \to 0 \\ \mu \to 0}}{Lt} \left[\frac{d^2 I_1}{\delta\lambda\, \delta\mu} - \frac{d^2 I_1}{\delta\lambda\, \delta\eta}\right], \tag{7}$$

where
$$\begin{aligned} I_1 = {} & \left[1/(2\pi i)^3\right] \oint\oint\oint dt_1 dt_2 dt_3\, t_1^{i\alpha_1 - 1}(t_1 - 1)^{-i\alpha_1} \\ & \times t_2^{i\alpha_2 - 1}(t_2 - 1)^{-i\alpha_2}\, t_3^{-i\alpha_3 - 1}(t_3 - 1)^{i\alpha_3} \times J,\end{aligned} \tag{8}$$

with
$$\begin{aligned} J = {} & \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \exp\left[-\lambda r_2 + i\{(\boldsymbol{k}_i - \boldsymbol{k}_1).\boldsymbol{r}_1 - \boldsymbol{k}_2.\boldsymbol{r}_2 + (k_1 r_1 + \boldsymbol{k}_1.\boldsymbol{r}_1)t_1\right. \\ & \times (k_2 r_2 + \boldsymbol{k}_2.\boldsymbol{r}_2)t_2 + (q r_{12} + \boldsymbol{q}.\boldsymbol{r}_{12})t_3\}]/(r_1 r_2 r_{12}).\end{aligned} \tag{9}$$

We first evaluate J using Fourier transformation technique [5] and then carry out the contour integrations over t_1, t_2 and t_3 in eq. (8).

Finally, we get

$$I_1 = 8\int d\boldsymbol{p} A^{-1+i\alpha_1}(A - B)^{-i\alpha_1} C^{-1+i\alpha_2}(C - D)^{-i\alpha_2} E^{-1-i\alpha_3}(E - F)^{i\alpha_3}, \tag{10}$$

where
$$A = (p+k_0-k_1)^2+\eta^2;\ A-B=(P+k_0)^2+(\eta-ik_1)^2;$$
$$C=(P+k_2)^2+\lambda^2;\ C-D = p^2+(\lambda-ik_2)^2; \tag{11}$$
$$E=p^2+\mu^2;\ E-F=(p-q)^2+(\mu-iq)^2;$$

A, C, E are all positive.

Performing the differentiations and taking the limits as stated in eq. (7), we have, after putting $\lambda = 1$:

$$I = -32\int dp\, F(p) f_{\alpha_2}(p)\left[f_{\alpha_1}(p)f_{\alpha_3}(p) + 2f'_{\alpha_1}(p)f'_{\alpha_3}(p)\right], \tag{12}$$

where

$$\left.\begin{aligned}
F(p) &= p^2 + p\cdot k_2 + ip\cdot\hat{k}_2,\\
f_{\alpha_2}(p) &= \left[(p+k_2)^2 + 1\right]^{-2+i\alpha_2}\left[p^2 + (1-ik_2)^2\right]^{-1-i\alpha_2},\\
f_{\alpha_1}(p) &= \left[(p+k_0-k_1)^2\right]^{-1+i\alpha_1}\left[(p+k_0)^2 - k_1^2 - i0_+\right]^{-i\alpha_1},\\
f'_{\alpha_1}(p) &= \left[(p+k_0-k_1)^2\right]^{-1+i\alpha_1}\left[(p+k_0)^2 - k_1^2 - i0_+\right]^{-1-i\alpha_1},\\
f_{\alpha_3}(p) &= \left[p^2\right]^{-1-i\alpha_3}\left[(p-2p\cdot q-i0_+)\right]^{-1+i\alpha_3},\\
f'_{\alpha_3}(p) &= \left[p^2\right]^{-1-i\alpha_3}\left[(p^2\cdot 2p\cdot q-i0_+)\right]^{i\alpha_3}.
\end{aligned}\right] \tag{13}$$

With the substitution $2q.\hat{p} = X$, the term $p^2 - 2p\cdot q - i0_+$ becomes $p(p-X-i0_+)$. In the small region where $p < X$, on account of the negative imaginary infinitesimal phase $-i0_+$, one can write

$$\left(p^2-2p\cdot q-i0_+\right)^{-n+i\alpha_3} = (-1)^n\exp(\pi\alpha_3)p^{-n+i\alpha_3}(X-p)^- \tag{14}$$

It is evident that the factor $\exp(-\pi\alpha_3)$ present in eq. (5) will be compensated for by the factor $\exp(\pi\alpha_3)$ of eq. (14). Hence in eq. (12), the contribution from this region only will be significant. The contribution to the matrix element from the rest of the momentum space will be vanishingly small due to the presence of the factor $\exp(-\pi\alpha_3)$.

Over the above mentioned significant small region $p^2 = 0(q^2)$, $p\cdot k_2 = 0(q\cdot k_2)$ and $p\cdot\hat{k}_2 = 0(q.\hat{k}_2)$, hence we need to consider only the term $ip.\hat{k}_2$ in $F(p)$ of eq. (13) which has the dominant contribution. Further $f_{\alpha_1}(p)$, $f'_{\alpha_1}(p)$ and $f_{\alpha_2}(p)$ of the same equation may be treated as constants over this small region and as such taken outside the integral. Moreover, the contribution to the integral from the term containing $f'_{\alpha_3}(p)$ is found to be insignificant and we consider only the part involving $f_{\alpha_3}(p)$.

We now choose the z-axis along q and take plane containing q and k_2 as the xz plane. Performing the integration over the azimuthal angle and writing $\cos\theta = Z$, we have

$$I = 64\, i\,\pi\cos(\hat{q}\cdot\hat{k}_2)\exp(\pi\alpha_3)\times C_p\times I', \tag{15}$$

where $C_p = \exp(-2) \times \exp(-2i\hat{k}_0 \cdot \hat{k}_1)$

and $$I' = \int_{\varepsilon'}^{2q} p^{-i\alpha_3}\, dp \int_{p+\varepsilon}^{2q} ZdZ(2qZ-p)^{-1+i\alpha_3}; \quad \varepsilon, \varepsilon' \to 0_+.$$

Integration with respect to Z yields

$$I' = \left[1/(2q)^2\right] \int_{\varepsilon'}^{2q} dp\, p^{-i\alpha_3} \left[\frac{(2q-p)^{i\alpha_3+1}}{i\alpha_3+1} + \frac{p(2q-p)^{i\alpha_3}}{i\alpha_3} - \frac{p\varepsilon^{i\alpha_3}}{i\alpha_3}\right]$$

In view of the fact

$$\underset{\varepsilon'\to 0_+}{Lt} \int_{\varepsilon'}^{2q} dp\, p^{m-i\alpha_3} (2q-p)^{n+i\alpha_3} = (2q)^{m+n+1} B(m+1-i\alpha_3, n+1+i\alpha_3)$$

which is proportional to $\exp(-\pi\alpha_3)$, we have after p integration, the final expression for the matrix element M,

$$M = 128\, i \left(\frac{\alpha_1 \alpha_2 \alpha_3}{\pi}\right)^{1/2} \times \exp(-2) \times \exp(-2i\hat{k}_0 . \hat{k}_1) \cos(\hat{q} . \hat{k}_2)$$
$$\times\, q^2 (\varepsilon/2q)^{i\alpha_3} \qquad (16)$$

It should be noted that the factor $\exp(-\pi\alpha_3)$ on account of the normalisation has been ultimately compensated for, which is a new and significant result.

Finally, since the cross section is proportional to $|M|^2$, it does not depend on the cut-off ε.

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